MSE3114: FUNDAMENTALS OF SCIENTIFIC COMPUTING: A COURSE POWERED BY AI

Effective Term
Semester B 2024/25

Part I Course Overview

Course Title
Fundamentals of Scientific Computing: a Course Powered by AI

Subject Code
MSE - Materials Science and Engineering
Course Number
3114

Academic Unit
Materials Science and Engineering (MSE)

College/School
College of Engineering (EG)

Course Duration
One Semester

Credit Units
3

Level
B1, B2, B3, B4 - Bachelor's Degree

Medium of Instruction
English

Medium of Assessment
English

Prerequisites
MA2158 Linear Algebra and Calculus or
MA2001 Multi-variable Calculus and Linear Algebra or
MA2172 Applied Statistics for Sciences and Engineering or
MA2177 Engineering Mathematics and Statistics or
MA2181 Mathematical Methods for Engineering

Precursors
Nil

Exclusive Courses
PHY3115 Introduction to Computational Physics

Part II Course Details

Abstract

Scientific computing is a discipline that focuses on solving scientific problems using computer-based approaches. The emphasis is placed upon utilizing software packages and the development of programming skills to address mathematical, physical, and materials engineering challenges. This course covers problem formulation, simulations and modelling, mathematical and numerical analysis, visualisation through graphics, introductory programming, and the utilization of artificial intelligence.

In this course, students will learn how to use Python programming and AI for solving scientific problems. Prior programming experience is not required, as the emphasis of the course is on problem-solving rather than programming. The course targets scientific problems in physics and materials engineering, aiming to introducing the use of computers in science to students who may need such skills in the pursuit of a major in Applied Physics or Materials Engineering.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Analyse and formulate the mathematical models for typical problems in Physics and Materials Engineering with aid of AI.		x	x	
2	Solve mathematical, physical, and materials engineering problems using programming (including the use of variables, arrays, matrices, and control structures) and computational packages (e.g., NumPy and SciPy). Write Python codes with aid of AI.		x	x	x
3	Implement fundamental numerical methods by Python programming, e.g., numerical root finding, solving ordinary differential equations, fast Fourier transform, etc.		x	x	
4	Analyse how numerical computation may lead to misleading results (including models being invalid and numerical errors).		x		

A1: Attitude
Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability
Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to real-life problems.

A3: Accomplishments
Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

Learning and Teaching Activities (LTAs)

	LTAs	Brief Description	CILO No.	Hours/week (if applicable)
1	Lecture	Students will engage in formal lectures to gain knowledge about basic Python programming, practical application of AI, fundamental numerical methods for scientific computing, problem formulation, and error analysis.	1, 2, 3, 4	3 hrs/wk
2	Tutorials	Students will engage in tutorial activities to apply the knowledge gained from the lectures to solve the practical problems by programming (with aid of AI) and to present the results by graphics.	1, 2, 3, 4	1 hr/wk

Assessment Tasks / Activities (ATs)

	ATs	CILO No.	Weighting (%)	Remarks (e.g. Parameter for GenAI use)
1	Assignments (At least 5)	1, 2, 3, 4	20	Allow use of CityU GPT Chatbot
2	Midterm Tests	1, 2, 3, 4	30	Allow use of CityU GPT Chatbot
3	Examination	1, 2, 3, 4		Duration: 2 hours. Allow use of CityU GPT Chatbot

Continuous Assessment (%)

50

Examination (%)

50

Examination Duration (Hours)

2

Assessment Rubrics (AR)

Assessment Task

1. Assignments

Criterion

1.1 Students can analyse and formulate the mathematical models for the physical and materials engineering problems. They can solve the problems and implement numerical methods by Python programming with aid of AI.

Excellent (A+, A, A-)

High

Good (B+, B, B-)

Significant

Fair (C+, C, C-)
Moderate

Marginal (D)
Basic

Failure (F)
Not even reaching marginal levels

Assessment Task
2. Midterm Tests

Criterion
2.1 Students can explain the basic concepts, perform error analysis, and write codes to solve basic mathematical and physical problems (with aid of AI).

Excellent (A+, A, A-)
High

Good (B+, B, B-)
Significant

Fair (C+, C, C-)
Moderate

Marginal (D)
Basic

Failure (F)
Not even reaching marginal levels

Assessment Task
3. Examination

Criterion
3.1 Students can explain the basic concepts, perform error analysis, and write codes to solve practical, comprehensive physical and materials engineering problems (with aid of AI).

Excellent (A+, A, A-)
High

Good (B+, B, B-)
Significant

Fair (C+, C, C-)
Moderate

Marginal (D)
Basic

Failure (F)

Not even reaching marginal levels

Part III Other Information

Keyword Syllabus

Introduction

How to solve a problem?

How to use CityU GPT chatbot?

Basic programming

Python

Linear algebra by NumPy, visualisation by matplotlib, and symbolic calculation by SymPy

Least squares fitting and brief introduction to machine learning

Systems of linear equations

Fixed-point problem: Banach theorem

Root-finding problem: Newton’ s method, damped Newton method, quasi-Newton method

Ordinary differential equations

Initial value problem: forward/backward Euler method, Heun method, Runge-Kutta method

Boundary value problem: shooting method, finite difference method

Fourier analysis

Continuous/discrete Fourier transform, fast Fourier transform

Introduction to parallel computing (tentative)

Reading List

Compulsory Readings

	Title
1	Lecture notes
2	Tutorial questions
3	Qingkai Kong, Timmy Siauw, and Alexandre Bayen (2020). Python Programming and Numerical Methods: A Guide for Engineers and Scientists. Academic Press

Additional Readings

	Title
1	Robert Johansson, Numerical Python: Scientific Computing and Data Science Applications with Numpy, SciPy and Matplotlib, 2nd ed., Apress, 2019.
2	Tobin A. Driscoll and Richard J. Braun, Fundamentals of Numerical Computation, Society for Industrial and Applied Mathematics, 2018.
3	Rainer Kress, Numerical Analysis, Springer, 1998.